

Marshall-Peierls sign rule for excited states of the frustrated J_1 - J_2 Heisenberg antiferromagnet

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Abstract

We present analytical and numerical calculations for some excited states of the frustrated J_1 - J_2 spin- $\frac{1}{2}$ Heisenberg model for linear chains and square lattices. We consider the lowest eigenstates in the subspaces determined by the eigenvalue M of the spin operator S_{total}^z . Because of the reduced number of Ising basis states in the subspaces with higher M we are able to diagonalize systems with up to $N = 144$ spins. We find evidence that the Marshall-Peierls sign rule survives for a relatively large frustration parameter J_2 .

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1 Introduction

We study the Marshall-Peierls sign rule (MPSR) for the frustrated spin- $\frac{1}{2}$ Heisenberg antiferromagnet

$$\hat{H} = J_1 \sum_{\langle NN \rangle} \mathbf{S}_i \mathbf{S}_j + J_2 \sum_{\langle NNN \rangle} \mathbf{S}_i \mathbf{S}_j, \quad (1)$$

where $\langle \text{NN} \rangle$ and $\langle \text{NNN} \rangle$ denote nearest-neighbor and next-nearest-neighbor bonds on a linear chain or a square lattice.

According to Marshall's early work in 1955 [1] we know the relative phases of the Ising basis states building the ground state wave function of a bipartite spin- $\frac{1}{2}$ Heisenberg antiferromagnet (MPSR, for more details see below). Later on Lieb and Mattis generalized the theorem to arbitrary site spins and bipartite lattices without translational symmetries [2, 3]. The knowledge of the sign is of great importance for the construction of variational wave functions (see e.g. [4]) and for quantum Monte Carlo procedures which may have the so-called minus-sign problem if the MPSR is violated (see e.g. [5]). In particular, the possible violation of the MPSR in frustrated systems is a serious problem for variational and quantum Monte Carlo procedures.

For the considered model (1) the MPSR can be proved for $J_2 \leq 0$. In the frustrated model ($J_2 > 0$) the MPSR can be destroyed [4, 6, 7]. However, in a recent work [4, 7] we have presented general arguments that the MPSR may survive for relatively large J_2 . These arguments are based on exact diagonalization results for small clusters (number of sites $N \leq 24$), as well as on the spin wave approximation. Following these arguments Zeng and Parkinson [8] use the MPSR as a new way of investigating the spatial periodicity in the ground state of frustrated spin chains. Furthermore, they studied the breakdown of the MPSR as a function of the chain length and the frustrating J_2 . By finite size extrapolation they estimated a finite critical value for J_2 for an infinite chain of about $0.03J_1$ where the MPSR is violated in the ground state.

Because of the exponential growth of the number of basis states the direct numerical calculation of the singlet ground state is limited to small clusters and the conclusions obtained from small systems seem not to be quite reliable.

In this paper we exploit the observation that the MPSR holds not only for the singlet ground state but also for every lowest eigenstate in any subspace with higher quantum number $M \leq \frac{N}{2}$ of the z-component of the total spin. In these subspaces the number of basis states is reduced and it is possible to diagonalize much larger systems. With this data an approximation to the thermodynamic limit is more reliable. Below we present data up to $N \leq 144$ and we can conclude that the MPSR survives indeed a finite frustration J_2 at least for states with higher quantum numbers M .

2 Marshall Peierls sign rule

In the unfrustrated limit $J_2 = 0$ the lowest eigenstate of the Hamiltonian (1) in each subspace of fixed eigenvalue M of the spin operator S_{total}^z reads

$$\Psi_M = \sum_m c_m^{(M)} |m\rangle, \quad c_m^{(M)} > 0. \quad (2)$$

Here the Ising states $|m\rangle$ are defined by

$$|m\rangle \equiv (-1)^{S_A - M_A} |m_1\rangle \otimes |m_2\rangle \otimes \cdots \otimes |m_N\rangle, \quad (3)$$

where $|m_i\rangle$, $i = 1, \dots, N$, are the eigenstates of the site spin operator S_i^z ($-s_i \leq m_i \leq s_i$), $S_A = \sum_{i \in A} s_i$, $M_{A(B)} = \sum_{i \in A(B)} m_i$, $M = M_A + M_B$. The lattice consists of two equivalent sublattices A and B . $s_i \equiv s$, $i = 1, \dots, N$, are the site spins. The summations in Eq.(2) are restricted by the condition $\sum_{i=1}^N m_i = M$. The wave function (2) is not only an eigenstate of the unfrustrated Hamiltonian ($J_2 = 0$) and S_{total}^z but simultaneously of the square of the total spin \mathbf{S}_{total}^2 with quantum number $S = |M|$. Because $c_m^{(M)} > 0$ is valid for each m from the basis set (3) it is impossible to build up other orthonormal states without using negative amplitudes $c_m^{(M)}$. Hence the ground state wave function Ψ_M is nondegenerated.

For the lowest energy eigenvalues $E(S)$ belonging to the subspace M we have the Lieb-Mattis level-ordering

$$E(S) < E(S+1), \quad S \geq 0, \quad (4)$$

i.e. the ground state is a singlet. Note that this level ordering might be violated by frustration. However, a lot of numerical calculations show the same level ordering also for strongly frustrated systems [9, 10].

3 Analytic Solutions

Now we include frustration ($J_2 > 0$). In the subspace with maximum $M = N/2$ the MPSR is never violated in any dimension. Here the only possible state is the fully polarized ferromagnetic state which does not change with increasing J_2 .

In the next subspace $M = (N/2) - 1$ analytic solutions are found for linear chains and square lattices. In this subspace we deal with the so-called one-magnon state, where the wave function can be expressed as a Bloch-wave with a given \vec{k} .

Linear Chain - In this case the solution can be found by comparing the energies as a function of the wave vector \vec{k} .

$$E(k) = J_1 \left(\frac{N}{4} - 1 + \cos(k) \right) + J_2 \left(\frac{N}{4} - 1 + \cos(2k) \right) \quad (5)$$

with $\vec{k} = \frac{2\pi}{N}i$, $i = 0, \pm 1, \pm 2, \dots, +\frac{N}{2}$. The comparison of $E(\pi)$ and $E(\frac{2\pi}{N}(\frac{N}{2}-1))$ yields the equation for the critical J_2

$$J_2^c = J_1 \frac{1 + \cos \left[\pi \left(1 - \frac{2}{N} \right) \right]}{1 - \cos \left[2\pi \left(1 - \frac{2}{N} \right) \right]}. \quad (6)$$

In the limit $N \rightarrow \infty$ one obtains $J_2^c = \frac{1}{4}J_1$.

Square lattice - For small J_2 in the considered subspace the lowest energy is obtained for $\vec{k} = (\pi, \pi)$ and reads $E_1 = J_1(N - 8) + J_2N$. The corresponding eigenfunction fulfills the MPSR. For larger J_2 we have to distinguish between two cases: (a) If the number of spins in the sublattice $N/2$ is even we find a transition at $J_2 = (J_1/2)$ to a twofold degenerated ground state with $\vec{k} = (\pi, 0)$ or $\vec{k} = (0, \pi)$ with an energy $E_2 = J_1(N - 4) + J_2(N - 8)$. This state violates the MPSR, i.e. we have $J_2^c = \frac{1}{2}J_1$. Notice, that the eigenfunctions with $\vec{k} = (\pi, 0)$ or $\vec{k} = (0, \pi)$ fulfill the so-called product-MPSR [4]. (b) If the number of spins in the sublattice is odd (e.g. $N = 26$), the situation is more complicated. The energy levels cross each other for J_2^c slightly greater than $\frac{1}{2}J_1$.

4 Numerical Results

In subspaces with lower quantum numbers $M < (N/2) - 1$ we cannot find simple expressions for the eigenvalues and eigenfunctions. Hence, we present exact diagonalization data for $M \leq (N/2) - 2$. Using a modified Lanczos procedure we calculate in every subspace M the state with the lowest energy $E_0(M)$. Since the number of Ising basis states increases exponentially as $\binom{N}{N-M}$, one can calculate $E_0(M)$ for **all** $M = \frac{N}{2}, \dots, 0$ only for relatively small systems (in our case $N \leq 26$). However, in subspaces with larger M we are able to present data for N up to 144. In all cases we use periodic boundary conditions. Analyzing the eigenfunction with respect to the MPSR we can determine numerically the critical J_2^c where the MPSR is violated.

Linear Chain - In Fig.1 we show J_2^c as a function of $1/N$. For $M(N) = (N/2) - 1$ the analytic result is drawn. For the next $M(N) = (N/2) - 2$ the data show a similar behavior with the same critical value of $J_2 = \frac{1}{4}$ for $N \rightarrow \infty$. By considering the numerical data an analytic solution can be predicted

$$J_2^c = J_1 \frac{1 + \cos \left[\pi \left(1 - \frac{2}{(N-1)} \right) \right]}{1 - \cos \left[2\pi \left(1 - \frac{2}{(N-1)} \right) \right]}. \quad (7)$$

The following subspaces $M(N) = (N/2) - p$, $p > 2$ show a different behavior with different critical values for J_2 if $N \rightarrow \infty$. These critical values decrease for increasing p but evidently a finite region with a non-violated MPSR is preserved.

In Fig.2 the critical J_2^c is shown as a function of a renormalized $M_r = M(N)/(N/2)$ for small systems ($N = 8, \dots, 26$) over the full range of M_r . $M_r = 1$ is the ground state subspace for a ferromagnet and $M_r = 0$ for an antiferromagnet. The finite size extrapolation for the ground state with $M_r = 0$ yields a small but finite critical value $J_2^c \approx 0.03J_1$ which corresponds to the value estimated by Zeng and Parkinson in [8]. The monotonic decrease of J_2^c

with decreasing M_r indicates a finite region of a validity of the MPSR for all M_r .

Square lattice - In Fig.3 we show J_2^c as a function of $1/N$. Here the N dependence is less regular and a finite size extrapolation is much more difficult. This is mainly connected with the shape of the periodic boundaries. For some of the finite lattices the boundaries are parallel to the x- and y-axis (e.g. for $N = 4 \times 4, 6 \times 6, \dots, 12 \times 12$) whereas for other lattices the boundaries are inclined (e.g. $N = 18, 20, 32$, see e.g [11]). The impression of an oscillating behavior of J_2^c versus $1/N$ stems just from the alternation of parallel and inclined finite lattices. Nevertheless, it is evident that the critical J_2^c goes to a finite value for $N \rightarrow \infty$. An extrapolation to the thermodynamic limit for the antiferromagnetic ground state, i.e. subspace $M = 0$, is almost impossible for the square lattice. However, if we assume for $M = 0$ that the J_2^c is almost independent of $1/N$ for $N > 16$ (as it is suggested by Fig.3 and by spin wave theory) we could estimate from our data for $N = 10, 16, 18, 20$ a critical value of about $0.2 \dots 0.3$.

Fig.4 supports this estimation. Here the critical J_2^c is shown for different small lattices $N \leq 34$ as a function of M_r . It is seen that for $M_r \leq 0.6$ the critical J_2^c does not strongly depend on M_r (in contrast to the linear chain, where we have a monotonic decrease) and gives for all the lattices a value of about $0.3J_1$ for the antiferromagnetic ground state ($M_r = 0$).

5 Conclusion

For linear chains and square lattices we have shown, that in subspaces with large quantum number M of the spin operator S_{total}^z , the Marshall-Peierls sign rule is preserved up to a fairly large frustration parameter J_2^c .

Moreover, for linear chains the finite size extrapolation is quite reliable even for the singlet ground state and yields for **all** M a finite parameter region for J_2 where the MPSR is valid.

For square lattices we observe in general higher critical values J_2^c compared to linear chains. From this observation and from the extrapolation for subspaces with higher M we argue that for square lattices the MPSR is stable against a finite frustration in all subspaces, too.

6 Acknowledgments

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Figure 1: Linear chain: The critical value J_2^c where the MPSR breaks down versus $1/N$ for different M ($J_1 = 1$).

Figure 2: Linear chain: The critical value J_2^c where the MPSR breaks down versus M_r for different N ($J_1 = 1$).

Figure 3: Square Lattice: The critical value J_2^c where the MPSR breaks down versus $1/N$ for different M ($J_1 = 1$).

Figure 4: Square Lattice: The critical value J_2^c where the MPSR breaks down versus M_r for different N ($J_1 = 1$).

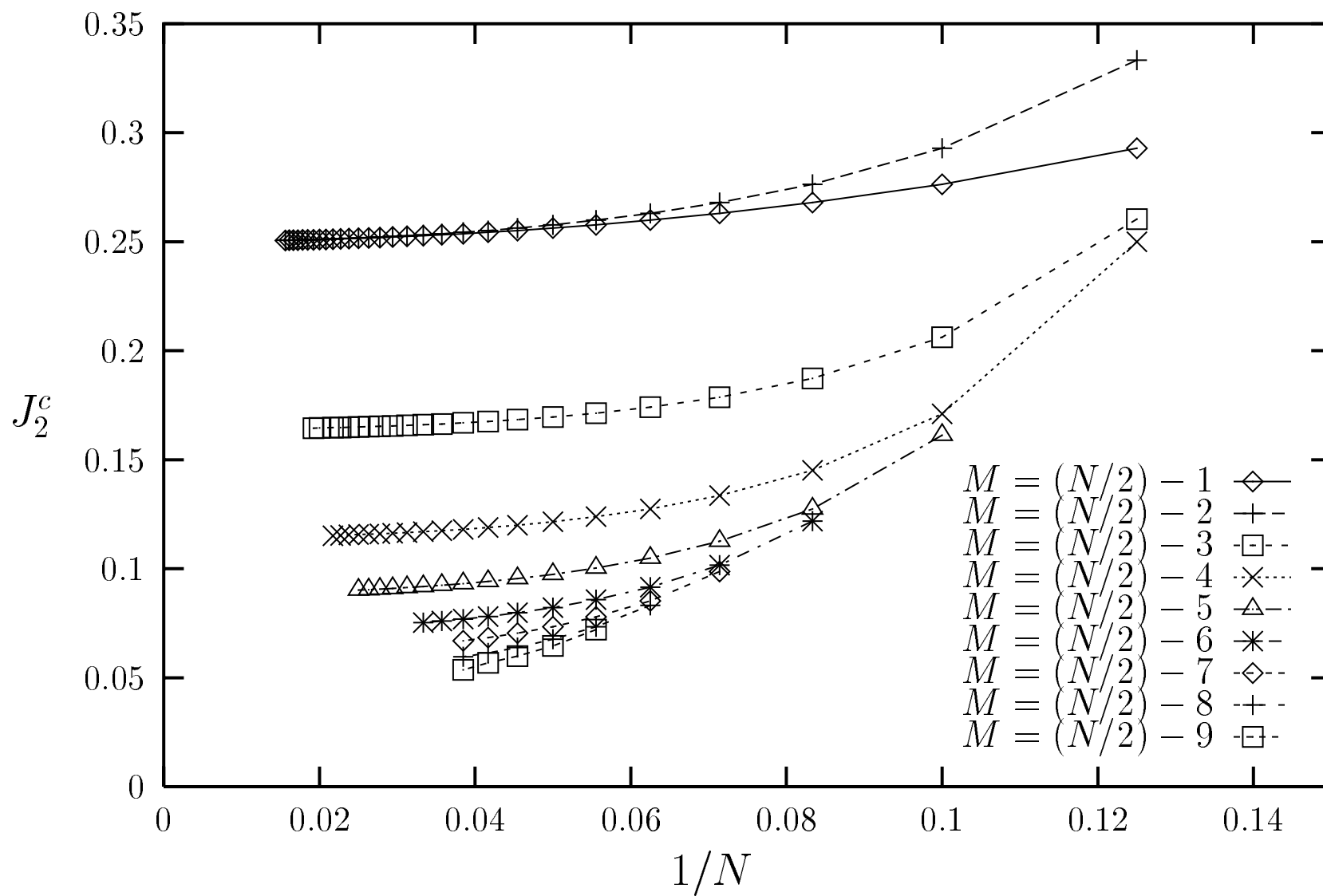


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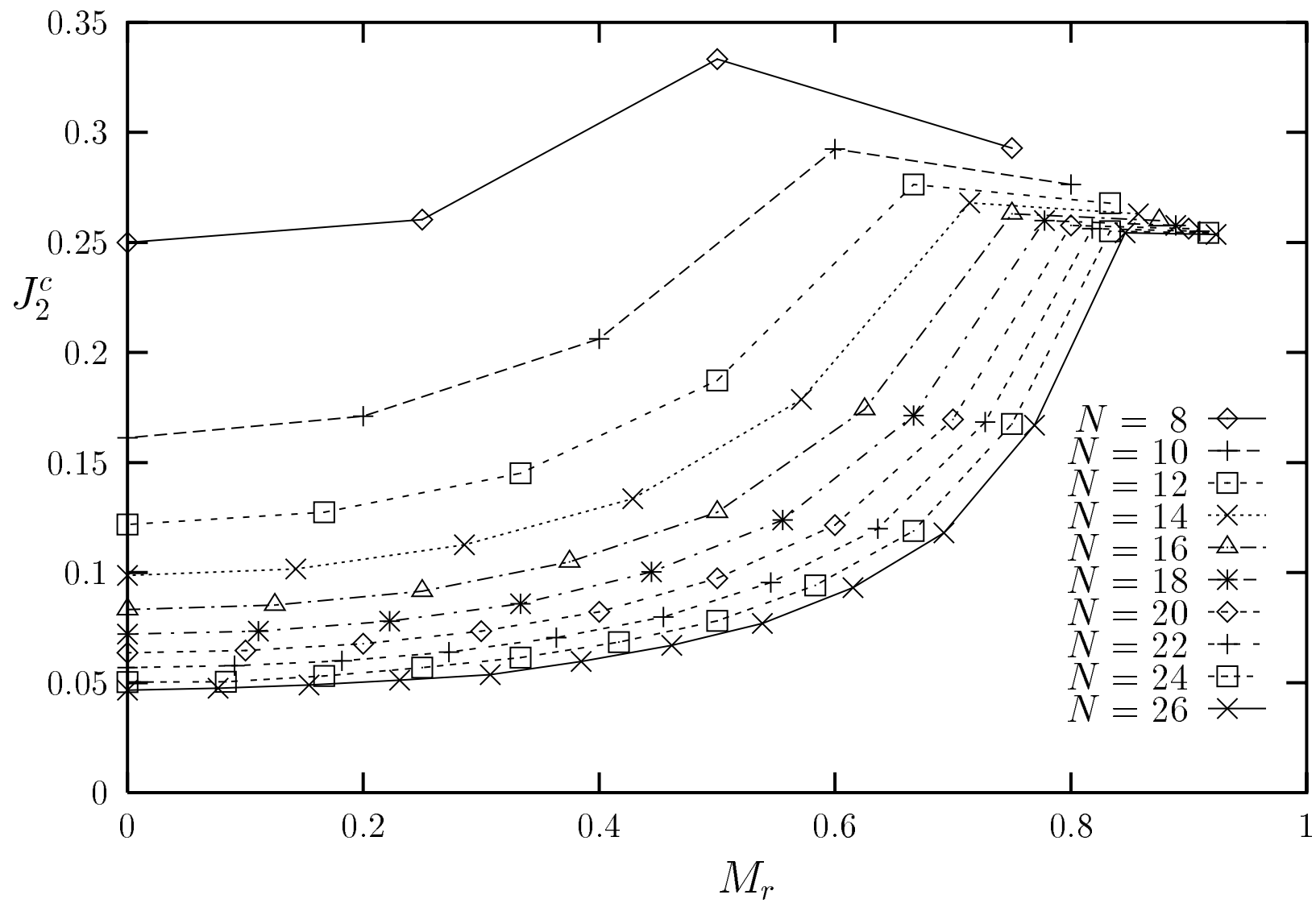


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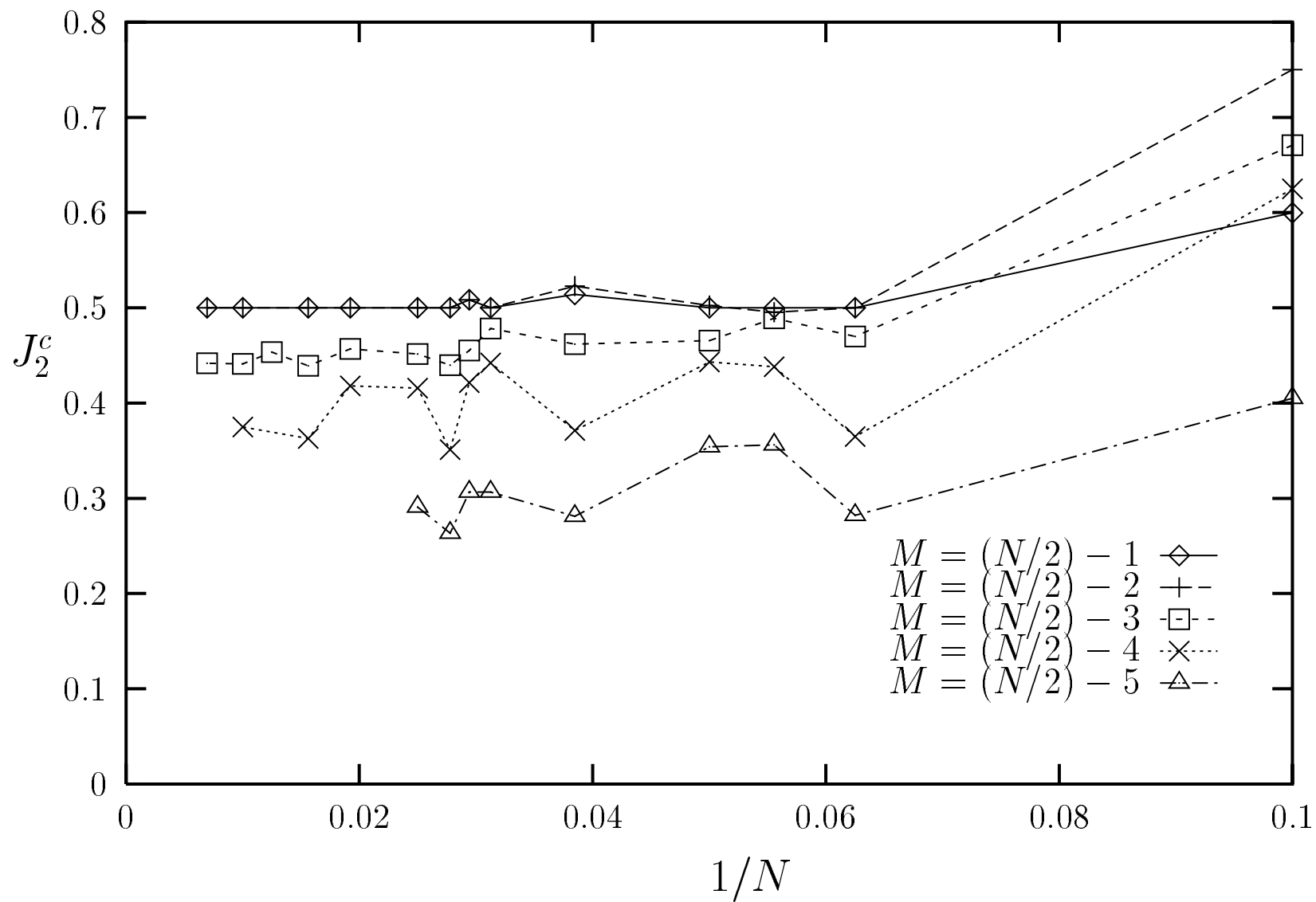


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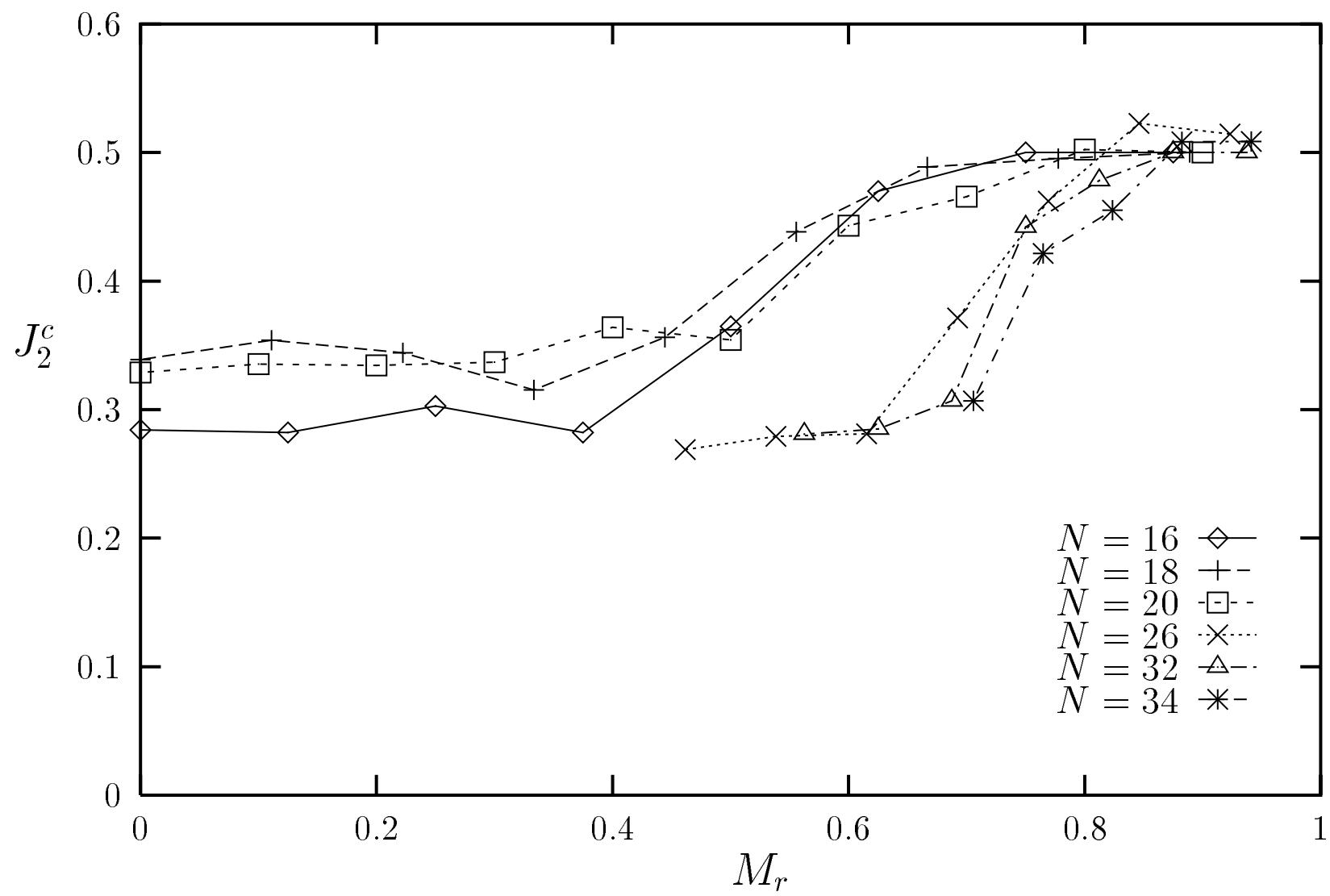


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